Time-dependent Bogoliubov–de Gennes and Ginzburg–Landau equations

Rupert L. Frank

LMU Munich

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Effective models

One wants to approximately describe complicated (quantum) many-body systems by simpler, effective models. The effective models involve typically only a single function in $\mathbb{R}^d$ (e.g., $d = 3$), whereas the original models involved functions on $\mathbb{R}^{dN}$.

Such an effective describtion is desirable both in static and dynamic problems.

Examples. (1) Schrödinger equation for bosons: Hartree theory, Gross–Pitaevski theory
(2) Schrödinger equation for fermions: Hartree–Fock theory, Vlasov equations

We approximate Hamiltonian systems by Hamiltonian systems.

Today's topic: Superconductivity
Microscopic description by Bardeen–Cooper–Schrieffer (BCS) (think: Hartree–Fock)
Macroscopic description by Ginzburg–Landau (GL) (think: NLS)

A relation between the micro and the macro description is possible in a static setting.

Question. Can one derive the time-dependent GL equations from time-dependent BCS equations (aka Bogoliubov-de Gennes (BdG) equations)?

$$id\partial_t\psi = -\Delta\psi + a\psi + b|\psi|^2\psi\,, \qquad a\in\mathbb{R}\,,\ b>0\,,\ \operatorname{Im} d \geq 0\,.$$

This equation is not Hamiltonian if $\operatorname{Im} d > 0$!

Answer. (=Main result for today) No! (generically)

The free Fermi gas at positive temperature

Reminder: Let $\mu \in \mathbb{R}$ (chemical potential) and $\beta > 0$ (inverse temperature).

$$\mathcal{A}^{(0)} := \left\{ \gamma \in L^1(\mathbb{R}^d, (1+|\xi|^2)d\xi) : \ 0 \leq \gamma \leq 1 \right\},$$

$$\mathcal{F}_\beta^{(0)}[\gamma] = \int_{\mathbb{R}^d} (|\xi|^2 - \mu)\gamma(\xi)\, d\xi + \beta^{-1} \int_{\mathbb{R}^d} \left(\gamma(\xi) \ln \gamma(\xi) + (1-\gamma(\xi)) \ln(1-\gamma(\xi))\right) d\xi \,.$$

The minimization problem

$$F_\beta^{(0)} := \inf_{\gamma \in \mathcal{A}^{(0)}} \mathcal{F}_\beta^{(0)}[\gamma]$$

has a unique minimizer, namely the Fermi–Dirac distribution

$$\gamma^{(\beta)}(\xi) = \left(1 + e^{\beta(|\xi|^2 - \mu)}\right)^{-1} \,.$$

In what follows, we will consider another minimization problem

$$F_\beta := \inf_{\Gamma \in \mathcal{A}} \mathcal{F}_\beta[\Gamma] \,,$$

where $\mathcal{A}^{(0)}$ can be considered as a subset of $\mathcal{A}$ and on this subset F_β coincides with $F_\beta^{(0)}$. The question is then whether the Fermi–Dirac distribution is still a minimizer.

The translation-invariant BCS functional

We denote by $\mathcal{A}$ the set of 2×2 matrix-valued functions on $\mathbb{R}^d$ such that

$$\Gamma(\xi) = \begin{pmatrix} \gamma(\xi) & \alpha(\xi) \\ \overline{\alpha(-\xi)} & 1 - \gamma(-\xi) \end{pmatrix}$$

with $\gamma \in L^1(\mathbb{R}^d, (1 + |\xi|^2) d\xi)$ and, for all $\xi \in \mathbb{R}^d$,

$$0 \leq \gamma(\xi) \leq 1, \qquad \alpha(\xi) = \alpha(-\xi), \qquad |\alpha(\xi)|^2 \leq \gamma(\xi)(1 - \gamma(-\xi))\,.$$

Note: We can identify $\mathcal{A}^{(0)}$ with those $\Gamma \in \mathcal{A}$ with $\alpha \equiv 0$.
Given a real, even function $V \in L^p(\mathbb{R}^d)$ ($p \geq 1$ if $d = 1$, $p > 1$ if $d = 2$ and $p > d/2$ if $d \geq 3$, plus always $p < \infty$), let

$$\mathcal{F}_\beta[\Gamma] = \int_{\mathbb{R}^d} (|\xi|^2 - \mu)\gamma(\xi)\, d\xi + \frac{1}{2} \int_{\mathbb{R}^d} V(x)|\check{\alpha}(x)|^2\, dx + \beta^{-1} \int_{\mathbb{R}^d} \operatorname{Tr} \Gamma(\xi) \ln \Gamma(\xi)\, d\xi\,.$$

Note: $\mathcal{F}_\beta[\Gamma] = \mathcal{F}_\beta^{(0)}[\gamma]$ if $\alpha \equiv 0$. Consider the minimization problem

$$F_\beta := \inf_{\Gamma \in \mathcal{A}} \mathcal{F}_\beta[\Gamma]\,.$$

Question: Is the minimizer of this problem equal to

$$\Gamma^{(\beta)}(\xi) := \begin{pmatrix} \gamma^{(\beta)}(\xi) & 0 \\ 0 & 1 - \gamma^{(\beta)}(\xi) \end{pmatrix} \quad ?$$

If yes: normal state, if no: superconducting state.

The critical temperature

The operator

$$K_\beta + V := \frac{-\Delta - \mu}{\frac{1}{2}\tanh\frac{\beta}{2}(-\Delta-\mu)} + V \qquad \text{in } L^2_{\rm symm}(\mathbb{R}^d)\,,$$

depends monotonically on β, and so do its eigenvalues. Therefore, there is a unique $\beta_c \in (0,\infty]$ such that

$$\inf \mathrm{spec}\,(K_\beta + V) < 0 \quad \text{for all } \beta > \beta_c\,, \qquad \inf \mathrm{spec}\,(K_\beta + V) \geq 0 \quad \text{for all } \beta \leq \beta_c\,.$$

Lemma (Hainzl–Hamza–Seiringer–Solovej)

$$F_\beta < F_\beta^{(0)} \quad \textit{for all } \beta > \beta_c\,, \qquad F_\beta = F_\beta^{(0)} \quad \textit{for all } \beta \leq \beta_c\,.$$

This is essentially a bifurcation result. The operator $K_\beta + V$ appears via the second variation of the function $\mathcal{F}_\beta$ around the normal state $\Gamma^{(\beta)}$.

Assumption

$$\beta_c < \infty \qquad \text{and} \qquad \dim\ker(K_{\beta_c} + V) = 1\,.$$

We choose $a_* \in \ker(K_{\beta_c} + V)$ with $\|a_*\|_{L^2(\mathbb{R}^d)} = 1$.

Derivation of Ginzburg–Landau theory

The following is a baby version of a much deeper result containing external fields.

Lemma (F.–Hainzl–Seiringer–Solovej)

$$F_\beta = F_\beta^{(0)} - e_*(\beta-\beta_c)^2 + \mathcal{O}((\beta-\beta_c)^{5/2}) \qquad \textit{as } \beta \searrow \beta_c\,.$$

Moreover, if Γ *satisfies* $\mathcal{F}_\beta[\Gamma] - F_\beta^{(0)} \leq (\beta-\beta_c)^2(-e_* + \epsilon)$ *with* $\epsilon \lesssim 1$*, then*

$$\alpha = \langle \widehat{a_*}, \alpha \rangle\, \widehat{a_*} + \zeta$$

with

$$|\langle \widehat{a_*}, \alpha \rangle| \lesssim (\beta-\beta_c)^{1/2}\,, \qquad \|\zeta\|_{L^2(\mathbb{R}^d)} \lesssim \beta-\beta_c\,.$$

$$\left|(\beta-\beta_c)^{-1}\,|\langle \widehat{a_*}, \alpha \rangle|^2 - \rho_*\right| \lesssim (\beta-\beta_c)^{1/4} + \epsilon^{1/2}\,.$$

- We have explicit formulas for the constants $e_*, \rho_* > 0$ in terms of μ and V (and a_*).
- Intuitively,

  $$\mathcal{F}_\beta[\Gamma] - F_\beta^{(0)} = (\beta-\beta_*)^2\Big(-e_* + \big(|\psi|^2 - \rho_*\big)^2 + \mathcal{O}((\beta-\beta_c)^{1/2})\Big)\,, \quad \psi = \frac{\langle \widehat{a_*}, \alpha \rangle}{(\beta-\beta_c)^{1/2}}\,.$$

  The quantity $(|\psi|^2 - \rho_*)^2$ is the Ginzburg–Landau functional.

The time-dependent problem

Time-dependent BdG equation

$$i\partial_t \Gamma(\xi) = [H_{\Delta_\Gamma}(\xi), \Gamma(\xi)] \, , \qquad \Delta_\Gamma(\xi) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} \widehat{V}(\xi - \xi')\alpha(\xi')\, d\xi' \, ,$$

where

$$\widehat{\Gamma}(\xi) = \begin{pmatrix} \gamma(\xi) & \alpha(\xi) \\ \overline{\alpha(\xi)} & 1 - \gamma(-\xi) \end{pmatrix}, \qquad H_\Delta(\xi) = \begin{pmatrix} |\xi|^2 - \mu & \Delta(\xi) \\ \overline{\Delta(\xi)} & \mu - |\xi|^2 \end{pmatrix}.$$

This is a Hamiltonian equation, which preserves the energy

$$\int_{\mathbb{R}^d} (|\xi|^2 - \mu)\gamma(\xi)\, d\xi + \frac{1}{2} \int_{\mathbb{R}^d} V(x)|\check{\alpha}(x)|^2\, dx \, ,$$

as well as the entropy

$$- \int_{\mathbb{R}^d} \operatorname{Tr} \Gamma(\xi) \ln \Gamma(\xi)\, d\xi \, .$$

Note that there is no temperature in the equation.

Question. Is there a $d \in \mathbb{C}$ (depending on V, μ and $\iota \in \{\pm 1\}$) with $\operatorname{Im} d \geq 0$ such that, if $0 < \iota(\beta - \beta_c) \lesssim h^2$ and if $\mathcal{F}_\beta[\Gamma_0] - F_\beta^{(0)} \lesssim h^4$, then the solution Γ_t of the BdG equation with initial condition Γ_0 satisfies, for any $t \in \mathbb{R}$,

$$\alpha_t \approx h\, \psi_t\, \widehat{a_*}$$

with ψ_t satisfying

$$id\partial_t \psi_t = -\iota \rho_* \psi_t + |\psi_t|^2 \psi_t \ ?$$

The time-dependent problem. Cont'd

Time-dependent BdG equation

$$i\partial_t \Gamma(\xi) = [H_{\Delta_\Gamma}(\xi), \Gamma(\xi)] \,, \qquad \Delta_\Gamma(\xi) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} \widehat{V}(\xi - \xi')\alpha(\xi')\, d\xi' \,,$$

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with ψ_t satisfying

$$id\partial_t \psi_t = -\iota\rho_* \psi_t + |\psi_t|^2 \psi_t \ ?$$

For $\iota = +1$ (so $\beta > \beta_c$) one expects $\operatorname{Im} d = 0$ and for $\iota = -1$ (so $\beta < \beta_c$) one expects $\operatorname{Im} d > 0$ ('superconductivity persist above β_c, but disappears below β_c').

This equation has been suggested in the physics literature (Stephen–Suhl (1964), Abrahams–Tsuneto (1966), Schmidt (1968)). This derivation was criticized by Eliashberg–Gorkov (1968), but it is still used successfully in theory and applications.

Main result

$$i\partial_t \Gamma(\xi) = [H_{\Delta_\Gamma}(\xi), \Gamma(\xi)] \,, \qquad \Delta_\Gamma(\xi) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} \widehat{V}(\xi - \xi')\alpha(\xi')\, d\xi' \,,$$

where

$$\widehat{\Gamma}(\xi) = \begin{pmatrix} \gamma(\xi) & \alpha(\xi) \\ \overline{\alpha(\xi)} & 1 - \gamma(-\xi) \end{pmatrix}, \qquad H_\Delta(\xi) = \begin{pmatrix} |\xi|^2 - \mu & \Delta(\xi) \\ \overline{\Delta(\xi)} & \mu - |\xi|^2 \end{pmatrix}.$$

Assumption

$$\mu > 0 \qquad \text{and} \qquad \sup_{|\xi|^2=\mu} |\widehat{a_*}(\xi)| > 0 \,.$$

Theorem (F.–Hainzl–Schlein–Seiringer)

Let Γ_t be a solution of the time-dependent BdG equation with initial data Γ_0. Then, if β is sufficiently close to β_c, we have, for all $t \in \mathbb{R}$,

$$\left| |\langle \widehat{a_*}, \alpha_t \rangle|^2 - |\langle \widehat{a_*}, \alpha_0 \rangle|^2 \right| \lesssim \max \left\{ |\beta - \beta_c|^{5/4}, \left(\mathcal{F}_\beta(\Gamma_0) - F_\beta^{(0)} \right)_+^{5/8} \right\}.$$

- We will see in the proof that, for all $t \in \mathbb{R}$,
  $$|\langle \widehat{a_*}, \alpha_t \rangle|^2 \lesssim \max \left\{ |\beta - \beta_c|, \left(\mathcal{F}_\beta(\Gamma_0) - F_\beta^{(0)} \right)_+^{1/2} \right\}$$
  which is order-sharp, so the theorem shows a cancellation in the difference.
- Thus, $t \mapsto |\langle \widehat{a_*}, \alpha_t \rangle|^2$ is constant to leading order in $\beta - \beta_c$, contradicting that a time-dependent GL equation with $\operatorname{Im} d > 0$ is satisfied.

Proof of the main result

Step 1. Structure of states with low free energy

Lemma

If $|\beta - \beta_c|$ is sufficiently small, then for any $\Gamma \in \mathcal{A}$

$$\gamma(\xi) = \frac{1}{1 + e^{\beta(|\xi|^2 - \mu)}} + \eta(\xi)\,, \qquad \alpha(\xi) = \langle \widehat{a_*}, \alpha \rangle\, \widehat{a_*}(\xi) + \zeta(\xi)$$

with

$$|\langle \widehat{a_*}, \alpha \rangle| \lesssim h\,, \quad \|\eta\|_{L^2(\mathbb{R}^d)} + \|\zeta\|_{L^2(\mathbb{R}^d)} \lesssim h^2\,, \quad h = \max\left\{ |\beta - \beta_c|^{\frac{1}{2}}, \left(\mathcal{F}_\beta(\Gamma) - F_\beta^{(0)}\right)_+^{\frac{1}{4}} \right\}.$$

This follows by variational arguments.

Step 2. Pointwise conservation of the spectrum

Recall that the equation reads $i\partial_t \Gamma(\xi) = [H(t,\xi), \Gamma(\xi)]$ with $H(t,\xi)$ Hermitian. Thus, for each $\xi \in \mathbb{R}^d$, the matrices $\Gamma_t(\xi)$, $t \in \mathbb{R}$, are unitarily equivalent to $\Gamma_0(\xi)$. Diagonalizing the matrices, we see that

Lemma

For any $\xi \in \mathbb{R}^d$, $t \mapsto (\gamma_t(\xi) - \frac{1}{2})^2 + |\alpha_t(\xi)|^2$ is constant.

Proof of the main result, cont'd

Step 3. We abbreviate

$$h := \max\left\{ |\beta-\beta_c|^{1/2}, \left(\mathcal{F}_\beta(\Gamma_0) - F_\beta^{(0)}\right)_+^{1/4} \right\}.$$

By conservation of energy and of entropy, we can apply Step 1 at each time and obtain

$$\gamma_t(\xi) = \frac{1}{1+e^{\beta(|\xi|^2-\mu)}} + \eta_t(\xi)\,, \qquad \alpha_t(\xi) = h\,\psi_t\,\widehat{a_*}(\xi) + \zeta_t(\xi)\,, \qquad \psi_t := h^{-1}\langle \widehat{a_*}, \alpha_t\rangle$$

with

$$|\psi_t| \lesssim 1\,, \qquad \|\eta_t\|_{L^2(\mathbb{R}^d)} + \|\zeta_t\|_{L^2(\mathbb{R}^d)} \lesssim h^2\,.$$

By Step 2,

$$\eta_t(\xi)^2 - \eta_0(\xi)^2 - (\eta_t(\xi)-\eta_0(\xi))\tanh\tfrac{\beta}{2}(|\xi|^2-\mu) = |\alpha_t(\xi)|^2 - |\alpha_0(\xi)|^2\,.$$

The left side, integrated over $\{\xi\in\mathbb{R}^d : \left||\xi|-\sqrt{\mu}\right| < \delta\}$, is $\lesssim h^4 + h^2\delta^{3/2}$.
The right side, integrated over the same set, is

$$\geq h^2 \left| |\psi_t|^2 - |\psi_0|^2 \right| \int_{||\xi|-\sqrt{\mu}|<\delta} |\widehat{a_*}(\xi)|^2\, d\xi - \mathrm{const.}\left(h^3\delta^{1/2} + h^4\right).$$

Recalling the assumption $\sup_{|\xi|^2=\mu} |\widehat{a_*}(\xi)| > 0$ and picking $\delta = h$, we obtain the claim. □

What went wrong in the physics literature arguments?

In the physics literature, the BdG equation is first linearized and the linear part of the time-dependent GL equation is derived. Then the nonlinearity is taken into account to lowest order.

When looking at the linearized problem there is a Fermi Golden Rule mechanism: The zero eigenvalue of $K_{\beta_c} + V$ turns into a resonance. The imaginary part of this resonance gives rise to the imaginary part of d. (We can reproduce the computations in the physics literature.)

An aside: FGR mechanism also appears in the problem of asymptotic stability of ground states of the NLS and in a series of works on 'a tracer particle in a Bose gas'.

The separate treatment of the linear and the nonlinear parts, however, is not rigorous. The equation is

$$i\partial_t \alpha = L\alpha - (\eta + \overline{\eta})\widehat{V\check{\alpha}}\,.$$

Away from $|\xi|^2 = \mu$ one has

$$\eta_t(\xi) - \eta_0(\xi) \approx -\frac{|\alpha_t(\xi)|^2 - |\alpha_0(\xi)|^2}{\tanh \frac{\beta}{2}(|\xi|^2 - \mu)}\,,$$

which looks quadratic in h, but for $|\xi|^2 \sim \mu$ one has

$$\eta_t(\xi) - \eta_0(\xi) \approx \left| |\alpha_t(\xi)|^2 - |\alpha_0(\xi)|^2 \right|^{1/2} \sim h\,|\widehat{a_*}(\xi)| \left| |\psi_t|^2 - |\psi_0|^2 \right|^{1/2},$$

which is linear in h.

Summary

- We have seen that under a generic assumption the time-dependent Ginzburg–Landau equation does not describe solutions of the Bogoliubov–de Gennes equation close to the critical temperature, even though this is natural in view of the results in the static case and this equation is frequently used in theory and applications.
- It remains a challenging open problem to unveil the relevant additional physical effects that are responsible for the possible emergence of a time-dependent GL equation.
- From a mathematical perspective, it would be interesting to study the simple translation-invariant BdG equation in more detail and, in particular, understand the behavior close to the Fermi surface $\{|\xi|^2 = \mu\}$.

THANK YOU FOR YOUR ATTENTION!